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ELECTRONIC AND STRUCTURAL PROPERTIES OF GRAIN BOUNDARIES IN Cz-GROWN SILICON BICRYSTALS

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Abstract. - The electronic properties of a low angle grain boundary in a silicon bicrystal are investigated by the conductance technique of Nicollian and Goetzberger. A continuous density of states is found. The crystallographic structure of this grain boundary is characterized by transmission electron microscopy. A comparison of results obtained by these two independent methods indicates that the charge in the boundary is caused by extrinsic dislocations.

1. Introduction. A great number of experimental techniques was used in the last years for the characterization of polycrystalline semiconductors. However the current understanding of grain boundaries (GB) in semiconductors still suffers from at least two facts:

a) There are only very few methods to evaluate the electronic parameters of the trap states located at the GB.

b) Nearly no attempts have been made so far to correlate the crystallographic and electronic structure of GB's.

In this contribution we want to show that the conductance method of Nicollian and Goetzberger [1] originally developed for the Si/SiO₂ interface, can be transferred to describe the behaviour of a single silicon GB. The electrically active GB is analyzed by electron microscopy. It will be shown that this combination of experimental techniques yields instructive insight into the role of the GB microstructure.

2. Sample preparation. Boron doped \( N_A = 1 \times 10^{15} \text{cm}^{-3} \) bicrystals are grown by a double seed Czochralski technique. The two seeds are tilted around \([110]\).

For the electrical characterization, samples of \( 12 \times 3 \times 0.4 \text{mm}^3 \) are cut, the GB bisecting the long edge \([2,3]\). Sections of the bicrystal adjacent to those for the electrical characterization are prepared for the electron microscope analysis. After grinding to \( \sim 50 \mu \text{m} \) the specimens are ion-milled until a hole appears that intersects the GB. High voltage electron microscopy (650 kV) permits inspection...
of the GB over a relatively long distance. A Siemens 102 (125 kV) is used for higher resolution. Due to the special orientation of the sections, the foils are expected to have their normal coinciding with the tilt axis of the GB and to contain the GB perpendicular to the surface.

3. Structural observations. The exact position of the rotational axis can be determined by the Kikuchi patterns of both grains. The axis is found to be located in the middle of the stereographic triangle about 16° off [110] towards ~[131], i.e. almost [29,45,10]. The boundary plane is asymmetrically situated between the two grains and shifted to near [121] in one grain. The angle of rotation is 7.8±0.3°.

Figure 1 shows a high resolution micrograph. The upper grain is oriented such that the electron beam is incident exactly along [110]. Second grain is imaged very kinematically. Apart from horizontal thickness fringes a fine structure with a repetition distance of 1.8 nm is visible along the GB. This structure can be attributed to the dislocation network making up this GB. A crude model for a [110] tilt boundary formed by two sets of dislocations with Burgers vectors of type 1/2 <011> yields a distance of ~2.5 nm.

Another feature of the boundary is documented by the faint 'semicircular' contrasts visible especially in the kinematically imaged grain. These contrasts and the pertaining structure in the boundary are more pronounced in Fig.2 where both grains are set for simultaneous excitation of the corresponding {220} diffraction vectors.

Figure 3 shows the GB at a smaller magnification and indicates a quasihomogeneous distribution of the extrinsic dislocations, at least over distances corresponding to the field of view, i.e. a few 10 μm. It should be noted that no indication is
Quasihomogeneous distribution of extrinsic dislocations. Upper grain two beam case, lower grain very kinematically. Also no lattice dislocations are observed.

4. Electrical measurements. Recently we have shown [2,3] that the zero bias dc conductance and the high frequency behavior of a single GB can be quantitatively explained by thermionic emission of majority carriers over a GB potential barrier created by charged trap states. The response of this charge to sub-bandgap light allows us to derive a density of states. The electrical measurements reported here analyze the response of the charge on an applied ac signal.

Figure 4 shows capacitance $C$ and conductance $G$ of the GB for various dc bias at 260K (ac oscillator level 10 mV). For frequencies $\omega < 10^6$ Hz the behavior of $C$ cannot be explained by the small signal response of the depletion layer widths (Fig.5). With this model the huge capacitance would lead to depletion layer widths of $\sim 1$ nm, incompatible with known trapped charge of $\sim 1 \times 10^{11}$ e/cm$^2$ (from high frequency capacitance). The behaviour of $C$ and $G$ will be briefly discussed here, details will be published elsewhere.

![Error bar valid for all curves from 30 to 300 Hz](image1)

![Error bar valid for all curves from 30 to 300 Hz](image2)

Fig.4. Capacitance $C$ and conductance $G$ for various bias values at 260 K.
The net thermionic current of holes from left to right in Fig.5 is:

\[ j_{th} = A^*T^2 \exp(-e\zeta/kT) \exp(-e\phi/kT) (1-\exp(-eU/kT)) \]  

(1)

For \( U = U_{dc} + \delta U_{ac} \); \( \phi = \phi_{dc} - \delta \phi \); \( eU_{dc} \gg kT \); \( \delta U_{ac} = \delta U + \phi = e \omega t \); \( \delta \phi = \delta U_{ac} \), the measured admittance \( Y_{th} = a_j \delta U_{ac} \), with \( \gamma = e/k A^*T \exp(-e\zeta/kT) \exp(-e\phi_{dc}/kT) \) can be shown to be:

\[ Y_{th} = \gamma \cdot \frac{\delta \phi}{\delta U_{ac}} \]  

(2)

Equation (2) shows that the current \( j_{th} \) is not determined by the ac voltage directly, but by the response of the barrier to the voltage. A phase lag between \( \delta \phi \) and \( \delta U_{ac} \) causes a capacitive thermionic current. The real and imaginary parts \( A_1, A_2 \) of the barrier can be calculated from charge \( Q \) and trapping current \( j_{SS} \):

\[ Q/e = \chi \phi^{1/2} + (\phi + U)^{1/2} \]  

(3)

\[ j_{SS} = Y_{SS} \delta \phi = (G_{SS} + jB_{SS}) \delta \phi \]  

(4)

Eq. 5 shows that the current \( j_{th} \) is not determined by the ac voltage directly, but by the response of the barrier to the voltage. A phase lag between \( \delta \phi \) and \( \delta U_{ac} \) causes a capacitive thermionic current. The real and imaginary parts \( A_1, A_2 \) of the barrier can be calculated from charge \( Q \) and trapping current \( j_{SS} \):

\[ a_1 = \frac{A_1}{B} = \frac{B_{SS} + B}{2} \]  

(5)

\[ a_2 = \frac{A_2}{B} = \frac{B_{SS}G_{SS}}{(B_{SS} + B)^2 + G_{SS}^2} \]

(5)

\[ B_{SS} + B = \omega C \]  

(5)

\[ B_{SS} + B = \omega (C + C) \]  

(5)

\[ C \text{ and } C \]  

(5)

The conductance \( G_{SS} \) can be extracted from (5) and (6) with the final result:

\[ G_{SS} = \gamma B_{SS} B / (G_{SS}^2 + B_{SS}^2) \]  

(7)

Equation (7) shows that \( G_{SS} \) can be calculated from conductance and susceptance of the thermionic current. \( G_{SS} \) may then be analysed using the well known methods of admittance spectroscopy from single crystals or MOS structures [1].

In Fig.6 values for \( G_{SS}/\omega \) evaluated with (7) from the data of Fig.4 are shown in comparison to theoretical \( G_{SS}/\omega \) characteristics for three different distributions of GB trap states over energy and space. Curve a) represents \( G_{SS}/\omega = C_{SS} \ln (1 + \omega^{2} \tau_{m}^{2}) \) for a single level, curve b) \( G_{SS}/\omega = (eN_{SS}/2\tau_{m}) \ln (1 + \omega^{2} \tau_{m}^{2}) \) for a density of states [5]. In both cases, time constant \( \tau_{m} \) and density of states \( N_{SS} \) could be derived from the maximum of the curve.

It can be seen that both curves do not fit the measured curve even closely. Time constant dispersion is far broader. The time constant \( \tau_{m} \) is related to thermal velocity \( <v_{th}> \), capture cross section \( \sigma_{th} \), grain carrier concentration \( p_{G} \) and the barrier height \( \phi_{B} \) by:

\[ \tau_{m} = \exp(e\phi_{B}/kT)/<v_{th}>^{\sigma_{th}}p_{G} \]  

(8)
Equation (8) shows that small fluctuations of \( \phi \) due to spatial fluctuations of charge lead to a dispersion of time constants and therefore broaden \( G_{SS}/\omega \). This was taken into account by Nicollian and Goetzberger in their paper about the Si/SiO\(_2\) interface by a statistical model of the fluctuations [1]. For the probability of potentials a Gaussian distribution \( P(\phi) \) was used.

\[
G_{SS}/\omega = eN_{SS}/2 \int \ln(1+\omega^2 \tau^2_m) P(\phi)/\omega \tau_m d\phi
\]

In the framework of this well introduced model \( N_{SS}, \sigma^2 \) and the standard deviation \( \sigma_S \) of the potential can be evaluated from exact solutions of the integral (9) [6,7]. We use the procedure given by Simonne [7] which requires the values of the measured \( G_{SS}/\omega \) at the maximum of the curve and at the frequency \( 5\omega_{max} \).

To test the applicability of the model the integral is then numerically calculated for the whole frequency range. The agreement over the wide frequency range (Fig.6) proves that the charge in the GB is distributed statistically over space and continuously in energy.

6. Minimum distance of charges at the GB. Analyzing the model of charge fluctuations in a general way, Brews [8] found the standard deviation \( \sigma_S \) to be related to the minimum distance of charges. This distance \( \lambda \) can be calculated for a GB by:

\[
\lambda = (e^2-1)^{-1/2} b,
\]

where \( b = \varepsilon\varepsilon_0/(C_{C+CS}), C_{CS} = eN_{SS} \) and

\[
a = 4\pi \sigma^2_S (\varepsilon\varepsilon_0)^2 (kT/e)^2/eQ
\]

We calculate from our data a bias-independent minimum distance of \( \lambda = 7.2 \text{ nm} \).

7. Density of states, capture cross section and standard deviation. For the energy range of \( E_V = 0.472 \text{ eV} \) to \( E_V = 0.536 \text{ eV} \) (corresponding to the bias values of Fig.1), the density of states increases from \( 7.8 \times 10^{10} / \text{ cm}^2 \text{ eV} \) to \( 1.3 \times 10^{11} / \text{ cm}^2 \text{ eV} \). The capture cross section is \( (2.5 \pm 0.5) \times 10^{-14} \text{ cm}^2 \). The standard deviation for all bias values is \( (1.8 \pm 0.5) \text{ kT/e} \) at the temperature of 260 K.

Conclusions. The electrical properties of the investigated GB can be analyzed in the framework of the model of potential fluctuations originally developed by Nicollian and Goetzberger [1] for the Si/SiO\(_2\) interface. It provides a description of the observed behavior of the conductance and capacitance in the frequency range 5-10\(^6\)Hz. Especially the observed broad dispersion of the time constants of trapping processes at the GB can be explained by a continuous density of states caused by charges distributed statistically in space. The attribution of a single level to the GB is not...
applicable. As in the case of the Si/SiO₂ interface the potential fluctuation model yields the density of states, Nₜₜ, the capture cross section, σₜ, and the standard deviation of potentials, σₜ.

This analysis permits the correlation of electronic properties with the crystallographic structure of the GB:

The standard deviation σₜ, as obtained from the potential fluctuation model, yields a minimum distance between the statistically distributed charges of 7±2 nm. The observations on the extrinsic dislocations are compatible with this analysis. They have an average distance of ~25 nm and are, contrary to the regular array of the narrowly spaced dislocations, irregularly distributed in the GB. This comparison thus leads to the conclusion that the charges are caused by and located at the extrinsic dislocations in the investigated grain boundary.

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References.

1 NICOLLIAN E.H., GOETZBERGER A., Bell Syst. Techn. J. 46 (1967) 1055
4 BALLUFFI R.W., KOMEM Y., SCHÖBER T., Surface Sci. 31 (1972) 68
7 SIMONNE J.J., Solid State Electron. 16 (1973) 121
8 BREWS J.R., J. Appl. Phys. 43 (1972) 2306